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Interfacial Pressures and Shocks in a Multiphase Flow Mix Model

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Abstract

Multiphase flow models have been proposed for use in situations which have combined Rayleigh-Taylor (RTI) and Richtmyer-Meshkov (RMI) instabilities [2, 3]. Such an approach works poorly for the case of a heavy to light shock incidence on a developed interface. I suggest that this difficulty can be overcome by adding an additional source to the turbulence kinetic energy equation. A variety of constraints on such a source are considered. In this context it is observed that a new constraint on closures arises. This occurs because of the discontinuity within the shock responsible for the RMI. The proposed model (Shock Scattering) is shown to give useful results.

1 Introduction

Multiphase flow models have been proposed for use in situations which have combined Rayleigh-Taylor (RTI) and Richtmyer-Meshkov (RMI) instabilities [2, 3]. Such an approach works poorly for the case of a heavy to light shock incidence on a developed interface. This may occur because of an inadequacy in the modeling of the sources to the k -equation. The situation is illustrated in a very schematic manner in Fig. 1. A shock interacting with a complex surface produces transmitted and reflected waves which cannot be represented by the mean flow \bar{u}_i . Note that these fluctuations $u_i'' =$

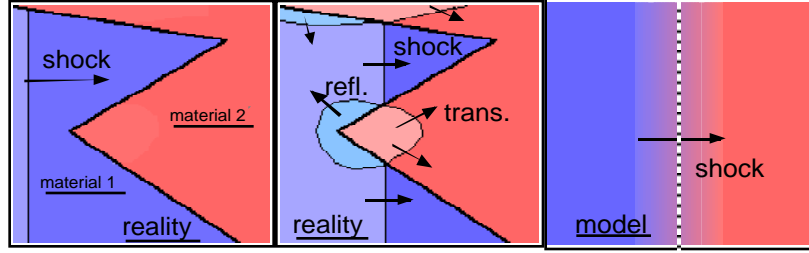


Figure 1: The figure shows a very schematic representation of the interaction of a shock with a mixed region. Part (a) is before the shock (incident from the left) interacts with the interface. Part (b) shows the interaction of the shock with the interface and the generation complex transmitted and reflected waves. Part (c) shows the view of this by the mix model.

$u_i - \tilde{u}_i$ between the actual complex velocity field u_i and the mean flow \tilde{u}_i arise from the interaction between the shock and the interfaces (or, more generally, between the shock and density gradients). They therefore represent a shock-mix interaction, and not a shock-turbulence interaction. I.e., these fluctuations will be generated even if initially $u_i'' = 0$. In many models fluid motions which cannot be represented by the mean flow are absorbed into a quantity like¹ $k = \frac{1}{2\rho} \cdot \overline{\rho u_i'' u_i''}$. If this is the case, then we should expect a source term in the time evolution equation for k of the form

$$\partial_t(\rho k) + \dots = \dots + E'(\text{shocks, mix}) \quad (1)$$

where E' depends on the presence of a shock and a mixed region, but not on the presence of velocity fluctuations. I.e., a term which does not vanish just because $k = 0$. Such a term may arise in the context of a multiphase flow model, and I propose that it be called “shock scattering.”

The balance of this paper will consist of 1) a motivation for the use of multiphase flow models, 2) a description of how interfacial pressure terms arise, 3) a consideration of the constraints on the modeling of these terms, 4) a description of an implementation of the model, and 5) the comparison of the model to three experiments which can be used to set some of the new parameters which have been added.

2 Motivation

Because this work relies heavily on the formalism used to derive the equations of multiphase flow [5], it is useful to review this so as to appreciate its applicability to the

¹This is the simplest case. One might also have multiple k 's for small and large scales, direction specific k 's to capture anisotropies in the flow, etc.

case of mixing² produced by a combination of the Rayleigh-Taylor and Richtmyer-Meshkov instabilities. In the presence of n materials or phases³ the mass or continuity equation must be split into n separate equations, one for each phase- r :

$$\partial_t \rho_r + \partial_{x_i}(\rho_r u_i) = 0, \quad \rho = \sum_r \rho_r \quad (2)$$

(The index i labels a direction and the index r labels a phase.) Note that this is simply the physics and *not* a modeling equation. It is valid at every point in space (trivially if the phase is not present). It contains only a single velocity u_i . This increase in complexity is required for the simple reason that one now needs to keep track of the locations of n different materials. Associated with these is a single (vector) momentum equation

$$\partial_t(\rho u_i) + \partial_{x_j}(\rho u_j u_i) = -\partial_{x_i} p \quad (3)$$

and an analogous equation for the internal energy.

The need for a model arises when the complexity of the flow makes the calculation of details of the interpenetration (mix) impractical or unnecessary. In such a case it is hopefully not necessary to know ρ_r at every point in space and time, but rather it is sufficient to know only an average value $\overline{\rho_r}$. The bar here denotes an averaging operation which is to be understood in an ensemble sense. (See reference [5].) The equation for the averaged quantity is obtained almost trivially

$$\partial_t \overline{\rho_r} + \partial_{x_i}(\overline{\rho_r u_i}) = 0 \quad (4)$$

where the second term illustrates the problem. This term contains an unknown correlation between the presence of the phase- r (ρ_r) and the velocity (u_i). Hence the problem of mix modeling reduces to that of modeling the correlation $\overline{\rho_r u_i}$.

As an aside it is useful to consider a path sometimes taken in mix modeling. One can define both an average density $\bar{\rho}$ and a mass weighted average velocity $\tilde{u}_i = \overline{\rho u_i} / \bar{\rho}$ without regard to the presence or absence of a particular phase. From this one can define a velocity fluctuation $u_i'' = u_i - \tilde{u}_i$ which makes it possible to write the previous equation as

$$\partial_t \bar{\rho} + \partial_{x_i}(\bar{\rho} \tilde{u}_i) = -\partial_{x_i}(\overline{\rho_r u_i''}) \quad (5)$$

Since the advection term on the left-hand side contains the same velocity for every phase, this term will not produce any mixing. The problem then reduces to modeling the correlation in the term on the right side $\overline{\rho_r u_i''}$.

At this point it is not uncommon to concede defeat by invoking a gradient diffusion closure. I.e., taking

$$\overline{\rho_r u_i''} = -D \partial_{x_i} \bar{\rho} \quad (6)$$

²In this paper I am going to use the term “mix” to mean the interpenetration of two (or more) fluids. The subsequent molecular mix is not considered.

³I am going to use the term “phase” in the balance of this paper only because it has been used in the past. The reader might just as well understand this as “material” or “component.”

where $D \propto \sqrt{kl}$, for instance. While a closure such as this has very definite practical advantages in its implementation, its utility for modeling instability driven mix is unproven. Given that it has its motivation in the ideas of isotropic turbulence and analogies to kinetic theory, it is not obvious that such a closure should be applicable to the present problem. Such closures are often accompanied by complicated turbulence models. (Perhaps to obscure the fact that the proponent gave up on the initial $\overline{\rho_r u_i''}$ term).

In any case a more reasonable path is to model the mass flux in question $\overline{\rho_r u_i}$ and then use it to define a *phase specific* mass averaged velocity $\tilde{u}_{r,i} = \overline{\rho_r u_i} / \overline{\rho_r}$. This results in a set of phase specific mass conservation equations (i.e., multiphase flow equations)

$$\partial_t(\overline{\rho_r}) + \partial_{x_i}(\overline{\rho_r \tilde{u}_{r,i}}) = 0 \quad (7)$$

Note that this procedure has closed these equations without introducing a closure approximation as such. This is a cute trick if one can produce an evolution equation for the velocity $\tilde{u}_{r,i}$. Such an equation can, in fact, be obtained as follows. If the momentum equation is valid at every point in space, then it is also valid in the phase- r . I.e.,

$$\underbrace{\partial_t(\rho u_i) + \partial_{x_j}(\rho u_j u_i) = -\partial_{x_i} p}_{\substack{\text{everywhere:} \\ \text{simple boundary conditions}}} \rightarrow \underbrace{\partial_t(\rho_r u_i) + \partial_{x_j}(\rho_r u_j u_i) = -\partial_{x_i} p}_{\substack{\text{within phase-}r: \\ \text{complicated boundary conditions}}} \quad (8)$$

where the two equations differ only in the presence of the subscript r on the density ρ_r on the right-hand equation. The cost of this is that while for the left-hand equation one has very simple boundary equations (i.e., at the edges of the box), for the right-hand equation one has to specify the boundary conditions between the phases. From averaging the right-hand equation one obtains[5]

$$\partial_t(f_r \rho_r \tilde{u}_i) + \partial_{x_j}(f_r \rho_r \tilde{u}_j \tilde{u}_i) = -f_r \partial_{x_i} p - \partial_{x_j}(f_r T_{r,ij}) + \overline{\partial_{x_i}(X_r) p} - p_r \partial_{x_i} f_r \quad (9)$$

where $p_r = \overline{X_r p}$, X_r is a characteristic function for phase- r which is 1 in phase- r and 0 elsewhere, the volume fraction $f_r = \overline{X_r}$ and $\rho_r = \overline{\rho_r} / f_r$. The first three terms in the equation are the analogues to the unaveraged terms in the momentum equation. The last three terms (on the right) arise from the averaging process. The first of these $\partial_{x_j}(f_r T_{r,ij})$ is analogous to the Reynolds stress which occurs in the usual Reynolds or Favre averaging. In this case it differs in that the velocity fluctuations are with respect to the phase specific mass averaged velocity $\tilde{u}_{r,i}$, and not with respect to the overall mass average velocity \tilde{u}_i .

The last two terms arise because the averaging operation was performed over only the phase- r and the average of the pressure gradient within the phase- r is not the same as the gradient of the average of the pressure[5]. These terms are typically modeled as drag between the two phases.

Before proceeding with this, it is worthwhile to consider whether anything was obtained from this exercise. The answer to this is an emphatic yes, as the model at this

point is able to produce mixing (and demixing) *without any closure approximations*. To see this, consider a simple problem with a constant pressure gradient $g_i = \partial_{x_i} p_r$ with the fluids initially at rest. Then the momentum equation initially reduces to

$$\partial_t(f_r \rho_r \tilde{u}_i) = -f_r g_i \quad (10)$$

From this it is clear that the acceleration of each phase- r will go like $\frac{1}{\rho_r}$. The subsequent velocity separation will result in either mixing or demixing depending on the sign of g_i and the initial conditions. Models based on this formalism are also inherently anisotropic and will provide a sort of automatic scale separation if a closure is included for the Reynolds stress (i.e., a k -equation, etc.). The costs of this are interfacial pressures to model and phase specific Reynolds stresses.

2.1 Drag may not be enough

As was indicated above, the interfacial pressures which appear in the momentum equation are typically modeled as drag between the phases. This may not be adequate in the presence of shocks. To see this it is useful to consider the Reynolds stress which appears in the momentum equation

$$T_{r,ij} = \frac{1}{f_r} \overline{X_r \rho u''_{r,i} u''_{r,j}} \quad (11)$$

From this one can obtain an equation for the energy not resolved in the $\tilde{u}_{r,i}$ if we proceed as follows. First, assume that all the anisotropies are handled by the mean flow variables $\tilde{u}_{r,i} = \overline{\rho_r u_i} / (f_r \rho_r)$.

If this is the case, then it is reasonable to define a phase specific turbulence kinetic energy

$$k_r = \frac{1}{2\rho_r} \sum_i T_{r,ii} \quad (12)$$

If we make the further assumption that all the phases have similar velocity fluctuations k_r , then one can, without loss of information, sum over the phases to define a total turbulence kinetic energy

$$k = \frac{1}{\rho} \sum_r f_r \rho_r k_r = \frac{1}{2\rho} \sum_{r,i} f_r T_{r,ii} \quad (13)$$

The usual manipulations starting from the momentum equation (along with the assumptions above) eventually produce

$$\begin{aligned} \partial_t(\rho k) + \partial_{x_i}(\tilde{u}_i \rho k) &= -T_{in} \sum_r f_r \partial_{x_i} \tilde{u}_{r,i} + \sum_r \partial_{x_i} \left(X_r \frac{1}{\rho} \overline{u''_{r,k} u''_{r,i} u''_{r,i}} \right) \\ &+ \underbrace{\sum_r \left[\sum_i \tilde{u}_{r,i} \left(\overline{p_r \partial_{x_i} X_r} - p_r \partial_{x_i} f_r \right) + \overline{p'_r (\tilde{u}_{r,i} + u''_{r,i}) \partial_{x_i} X_r} \right]}_{\text{surface pressure terms}} \end{aligned} \quad (14)$$

where the first line contains the terms analogous to the single material case and the second line contains the terms arising from the surface pressure terms in the momentum equation. (I have dropped some of the higher order non-surface terms.) The surface terms are obviously not small and have been modeled previously as sources of the energy lost from the velocity slip due to drag and added mass effects[2, 3]. Further, if a mixed region is initially at rest then $u''_{r,i} = 0$, and as a consequence $T_{in} = 0$ and similarly for the triple correlation. Hence, only the surface pressure term is available to generate k as is required according to the argument presented in the introduction. This appears plausible since neither the pressure nor the mean flow velocities which appear in this term vanish. The model for this will be called “shock scattering” as was explained in the introduction.

3 Shock Scattering

At this point it seems plausible that there should exist a pair of additional terms in the momentum equation and the k -equation. I.e., $E_{r,i}$ and E' as in

$$\begin{aligned}\partial_t(f_r \rho_r \tilde{u}_i) + \partial_{x_j}(f_r \rho_r \tilde{u}_j \tilde{u}_i) &= \cdots + E_{r,i} \\ \partial_t(\rho k) + \partial_{x_i}(\tilde{u}_i \rho k) &= \cdots + E'\end{aligned}$$

If this is the case, then the first step is to consider what constraints might exist on the forms of $E_{r,i}$ and E' . The list includes (at least): 1) Well behaved in the presence of shocks, 2) No constants with units introduced, 3) Invariant under a Galilean transformation, 4) Energy and momentum must be conserved, 5) Length scale does not enter the problem.

3.1 Well behaved in the presence of shocks

Substantial constraints are placed on the form of $E_{r,i}$ and E' (as well as any other term which is used in a mix model) by the requirement that these terms have meaningful behavior in the presence of discontinuous solutions (i.e., shocks). Recall that there are subtle issues when shocks form in any system of differential equations. The two derivatives ∂_x and ∂_t are not defined (in the usual sense) at a discontinuity. For systems of conservation laws this can be dealt with through the ideas of generalized functions and weak solutions[6]. I.e.,

$$\begin{aligned}\text{an equation like:} \quad \partial_t \rho + \partial_x Q(\rho) &= 0 \\ \text{is interpreted to mean:} \quad \int \int_R (\rho \partial_t \phi + Q(\rho) \partial_x \phi) &= 0\end{aligned}$$

where ϕ is an arbitrary test function with compact support on R , ρ is some density, and $Q(\rho)$ is some flux. For continuous ρ and $Q(\rho)$ these two equations are equivalent

and can be obtained from each other by integration by parts. If ρ or $Q(\rho)$ become discontinuous only the second equation actually has meaning. From these sorts of considerations one also obtains the jump condition $[\rho] \cdot U = [Q(\rho)]$ (where $[X]$ means the change in X across the shock). Because mix models do not generally appear in conservation form,⁴ the situation with respect to discontinuous solutions is very murky indeed.⁵ Nevertheless, it is clear that the issue of the interpretation of these models in the presence of shocks does not go away just because it has been ignored to date. This issue may become worse in the models than in the Euler equations because of the presence of higher order derivatives and/or products of derivatives.

One can, nevertheless, see that a simple necessary condition exists for these terms to have meaning in the presence of shocks. If one considers a potential closure E' which appears on the right-hand side of some time evolution equation (of ρk for instance)

$$\partial_t (\rho k) + \dots = \dots + E'$$

then a set of necessary conditions for this term to be meaningful in the presence of a shock is⁶

$$\int_{\text{shock}} E' dt = \begin{cases} \cdot \text{finite} \\ \cdot \text{non-zero} \\ \cdot \text{depends only on the jump conditions across the shock} \end{cases} \quad (15)$$

In general one can show that “good” terms “work” by using integration by parts to move the derivatives off the discontinuous functions (so to speak). For “bad” terms no such manipulations appear possible, and it seems to be necessary to introduce a particular continuous form for the step, do the integration explicitly, and then show that the result is not defined (and therefore “does not work”) as the step is allowed to become discontinuous. Since the latter is somewhat more transparent, it will be used throughout.

Consider a test function

$$u^{\natural} = u^{\natural}(x+ct) = \begin{cases} u_1 & \text{if } x+ct < 0 \\ u_1 + (x+ct)\frac{\Delta u}{\Delta} & \text{if } 0 < x+ct < \Delta \\ u_2 = u_1 + \Delta u & \text{if } \Delta < x+ct \end{cases} \quad (16)$$

i.e., a linear ramp in u which goes from u_1 to u_2 over an interval Δ and which propagates with a velocity c . (The superscript \natural is used to indicate a discontinuous function.) Then it is trivial to see that in the limit $\Delta \rightarrow 0$ a continuous function times the derivative of a discontinuous function is O.K.

$$\int_{\text{shock}} f \partial_x u^{\natural} dt \rightarrow f \frac{\Delta u}{c} \quad \text{An example of such a term is the pressure gradient in the momentum equation.} \quad (17)$$

⁴This has never happened to my knowledge.

⁵In general, one has to accept the possibility (if not exactly the certainty) that the answers will depend on both the differencing schemes used, and also possibly on both the particular spatial and temporal discretizations used. Hence, one can not really claim to be “solving” the equations in this case.

⁶The requirement that the result be non-zero is not strictly necessary, zero being a perfectly good number. However, in the current context such a term is not useful.

Several other terms also work. The product of a discontinuous function and the derivative of a discontinuous function is O.K.

$$\int_{\text{shock}} h^{\sharp} \partial_x u^{\sharp} dt \rightarrow \left(h_1 + \frac{\Delta h}{2}\right) \frac{\Delta u}{c} \quad \text{Like the } pdV \text{ term in the internal energy equation.} \quad (18)$$

The product of a continuous function and the n^{th} derivative of a discontinuous function also works

$$\int_{\text{shock}} f \partial_x^n u^{\sharp} dt \rightarrow (-1)^{n-1} \partial_x^{n-1} f \frac{\Delta u}{c} \quad (19)$$

There are also at least a couple of terms which do not work. The product of the derivatives of two discontinuous functions

$$\int_{\text{shock}} \partial_x g^{\sharp} \partial_x u^{\sharp} dt \rightarrow \frac{\Delta g \cdot \Delta u}{c \cdot \Delta} \rightarrow \infty \quad (20)$$

and the product of a discontinuous function and the second derivative of a discontinuous function

$$\int_{\text{shock}} g^{\sharp} \partial_x^2 u^{\sharp} dt \rightarrow -\frac{\Delta g \cdot \Delta u}{c \cdot \Delta} \rightarrow -\infty \quad (21)$$

are both undefined. This is roughly the equivalent of saying that there is no meaning to multiplying δ -functions. (Note that these two cases are also related by an integration by parts.) Note also that the first of these rules out the use of $\partial_x \rho \cdot \partial_x p$.

Some terms are zero. These are a couple of almost trivial examples. The integral over a shock of either a continuous or discontinuous function vanishes.

$$\int_{\text{shock}} f dt = \int_{\text{shock}} g^{\sharp} dt = 0 \quad (22)$$

The point here being that one requires a certain degree of singular behavior out of the term in order to get a non-zero contribution as the width of the shock goes to zero. More complicated terms can also be zero. For instance

$$\begin{aligned} \int_{\text{shock}} \partial_x (g^{\sharp} \partial_x u^{\sharp}) dt &= \int_{\text{shock}} \partial_x g^{\sharp} \partial_x u^{\sharp} + \int_{\text{shock}} g^{\sharp} \partial_x^2 u^{\sharp} \\ &= \frac{\Delta g \cdot \Delta u}{c \cdot \Delta} - \frac{\Delta g \cdot \Delta u}{c \cdot \Delta} = 0 \end{aligned} \quad (23)$$

Figure 2 shows a rather schematic representation of this potential source term. The point to appreciate is that one might have difficulties integrating this numerically and actually getting zero.

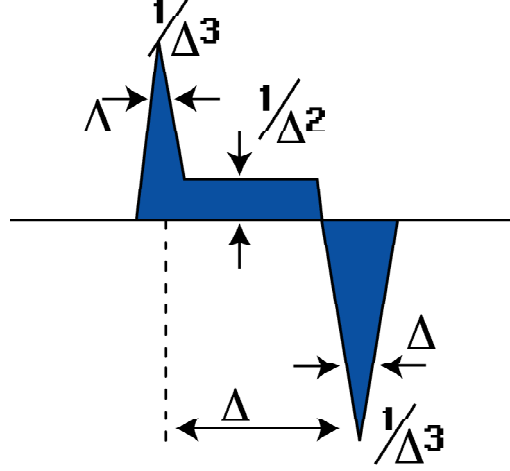


Figure 2: The figure shows the complex singular behavior of the term in eqn. 23. Labels show proportionality to Δ . This term, nevertheless, integrates to zero.

Terms which “do not work” are commonly used in turbulence modeling. Some of the terms indicated above which “do not work” are used in turbulence modeling in cases where there are typically no shocks. An example of such a situation is a common closure for the Reynolds stress[8].

$$\overline{\rho u_i'' u_i''} = T = - \underbrace{\mu_T \frac{4}{3} \partial_x u}_A + \underbrace{\frac{2}{3} \rho k}_B, \quad \mu_T = \rho \sqrt{k} l \quad (24)$$

The labels A and B will be used in the discussion below as these two parts of the closure behave in a very different manner in the presence of a shock. This term appears in both the momentum equation and in the equation for k , acting as a sort of turbulent pressure which can move energy between the mean flow and the unresolved scales k .

$$\begin{aligned} \partial_t (\rho u) + \dots = \dots - \partial_x T &= \dots \underbrace{\partial_x \left(\mu_T \frac{4}{3} \partial_x u \right)}_A - \underbrace{\frac{2}{3} \partial_x (\rho k)}_B \\ \partial_t (\rho k) + \dots = \dots - T \partial_x u &= \dots \underbrace{\mu_T \frac{4}{3} (\partial_x u)^2}_A - \underbrace{\frac{2}{3} \rho k \partial_x u}_B \end{aligned} \quad (25)$$

By the criteria given above the B terms “work.” The A terms do not. The A term in the k -equation contains the product of two derivatives of a discontinuous function, and

will make an undefined contribution to k .

$$\int_{\text{shock}} \mu_T \frac{4}{3} (\partial_x u)^2 dt = \rho \sqrt{k} l \cdot \frac{4}{3} \cdot \frac{(\Delta u)^2}{c \cdot \Delta} \propto \frac{1}{\text{zone size!}} \quad (26)$$

The corresponding A term in the momentum equation has no net effect on the momentum, but because it acts to accelerate and decelerate the flow at times at which the flow velocity is very different (recall the discontinuous change in u), it can nevertheless change the energy in the mean flow.

In any code, of course, shocks always have a finite width so that in practice “bad terms” as identified here will have large but finite effects due to shocks. In an Euler code (one with no explicit viscosity) these effects will be proportional to inverse powers of the zone size (since shocks are typically spread over a few zones by artificial viscous effects of one sort or another). This means that models with such terms will prevent the code from reaching a converged answer as the zone size is reduced. In a code with explicit viscous effects, “bad terms” will produce effects which depend upon the viscosity. As shock interactions are generally thought to be independent of the actual viscosity and thermal conductivity which determine the width of the shock[7] this would appear to be the wrong physics.

These observations are not entirely new. At least one author[9] understood that some of these terms get too big, and that limiters must be used. While anecdotal evidence suggests that the use of limiters may be more widespread and not generally reported in the literature[4, 10], it is not clear that the fundamentally undefined character of these terms has been appreciated. To put this another way, the difficulty here goes beyond the idea of realizability constraints[8].

Lastly, one should ask if there are any ways around the difficulties described in this section. If the model were to act upon the mean flow variables so as to induce a correct shock width (in the average sense), then all the “bad” terms would be defined. Such an interaction is expected in some sense, of course, because the Reynolds stress term in the momentum equation can have the form of a viscosity. The usual closure will presumably not work in the present case because it is (at best) a shock-turbulence interaction and not a shock-mix interaction. Even with a closure which induces the correct shock width, it might be a difficult task to get overall reasonable behavior. I.e., it is not clear that a “bad” term with a value of Δ proportional to the average shock width induced by the passage through a mix material would give reasonable behavior. Such a model would also require that the resolution in the simulation be adequate to resolve the shock width.

3.2 Influence of the Length Scale

Before turning our gaze upon the desperate cure of “dimensional analysis,” it is worthwhile to consider whether the length scale (i.e., the size of the large scale structures

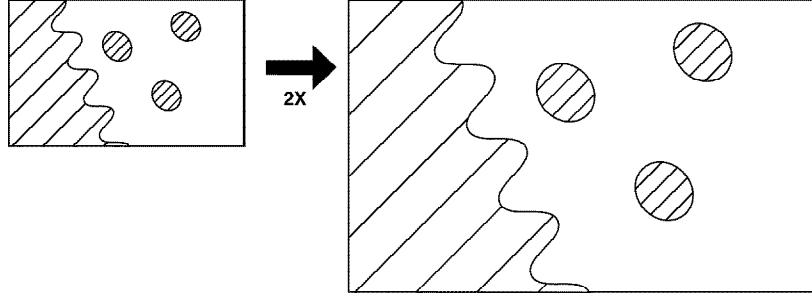


Figure 3: We consider what would happen if we change all the length scales in a shock mix region interaction by a factor of 2.

in the mix region) can reasonably enter into the term. Consideration of the microscopic shock interface interaction suggests that the length scale does not matter.⁷ More formally we can consider the similarity parameters in radiation hydrodynamics. We follow Pai [14], and consider a change in the length scale of the problem as is shown in Fig. 3. The length scale enters into the following parameters

$$\begin{aligned} \text{time parameter} \quad R_t &= \frac{U t_0}{L} \\ \text{Reynolds number} \quad R_e &= \frac{UL}{\nu_s} \\ \text{Radiation Knudson number} \quad L_{R^*} &= \frac{L_R}{L} \end{aligned}$$

(Here L is a characteristic material length, t_0 a characteristic time, U a characteristic velocity, and L_R a characteristic length for radiation diffusion.) Of these, L_{R^*} is clearly not relevant. We expect that R_e will also not be relevant on the short time scales it takes to produce the velocity fluctuations. Hence only the time parameter need concern us. If we scale the time by the same amount, then R_t is unchanged. Hence we expect to get exactly the same velocity field in the problem as long as we wait until the shock is in the analogous position.

It follows from this that we do **not** expect any factors of l in the term we are looking for. This is quite significant as it limits greatly the number of possible forms.

3.3 Dimensional analysis

The dependant variables in the model which are available for building the required term are as follows: $\rho_r, \tilde{u}_r, e_r, k, l$ plus the operator ∂_{x_i} . We do not consider ∂_t as it can always be removed using the time evolution equations. There exists an ambiguity with respect to the application of ∂_{x_i} , which will allow for multiple terms.

⁷I.e., the scattering of the shock at the interface occurs at an almost point-like region which does not “know” about the size of the structure.

We showed above that the length scale l does not enter. As we are searching for a term which will generate turbulence where there was none, no powers of k can appear in the term. Lastly, instead of using the internal energy e , we will substitute the pressure. As $p = p(\rho, e)$ this would appear to be general. For a polytropic gas $p = (\gamma - 1)\rho e$ and this is clearly the case.

Then the variables left at this point and their units are: $\rho[\text{m}/\text{l}^3]$, $u[\text{l}/\text{t}]$, $p[\text{m}/\text{lt}^2]$, and $\frac{\partial}{\partial x_i}[\text{l}/\text{l}]$. The required units come from $\frac{\partial}{\partial t}(\rho k)[\text{m}/\text{lt}^3]$. The form of the desired term is then

$$\rho^\alpha u^\beta p^\gamma \left(\frac{\partial}{\partial x_i} \right)^\delta \quad (27)$$

We can then write the following system of equations needed to get the units correct

$$\begin{pmatrix} \alpha & +\gamma & \\ -3\alpha & +\beta & -\gamma & -\delta \\ & \beta & +2\gamma \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 3 \end{pmatrix} \quad (28)$$

where the rows correspond to $[\text{m}]$, $[\text{l}]$, and $[\text{t}]$. The columns correspond to ρ , u , p , $\frac{\partial}{\partial x_i}$. Given 3 equations and 4 unknowns, we do not expect a unique solution. Nevertheless, δ is determined uniquely. To see this multiply the top equation by 3 and add it to the middle one. The resulting is $\beta + 2\gamma - \delta = 2$ which when combined with the third equation shows that $\delta = 1$.

The resulting three equations in three unknowns are not linearly independent, but we can write β and γ as functions of α . This gives

$$\rho^\alpha u^{1+2\alpha} p^{1-\alpha} \frac{\partial}{\partial x_i} \quad (29)$$

3.4 Invariance

It is well known that E' must be invariant under a change in coordinate systems. The term $u^{1+2\alpha}$ above might break such an invariance. This can be “fixed” either by taking the exponent of u to be zero so that $\alpha = -1/2$, or by taking the exponent to be one so that $\alpha = 0$ and letting the derivative operate on it. These two cases result in

$$\partial_t(\rho k) + \dots = C \cdot \sqrt{\frac{p}{\rho}} \partial_x p \quad \text{or} \quad \partial_t(\rho k) + \dots = C \cdot p \cdot \partial_x u \quad (30)$$

The left one being roughly a pressure gradient times a sound speed and the right one a $p\delta V$ work term.

3.5 Energy and momentum conservation

Lastly, the need to conserve momentum and energy forces the selection of the right-hand term. The total energy equation is obtained by multiplying the momentum equation in two forms by u and adding these to the equations for k and internal energy. Conservation is achieved if the combined term $\sum_r \tilde{u}_{r,i} \cdot E_{r,i} + E'$ either vanishes or forms a total divergence. The first of these would correspond to a purely local exchange of energy between the mean flow and k . The second case allows for energy transport as well as exchange. The first would require an inverse power of $\tilde{u}_{r,i}$ in the term in the momentum equation and, therefore, appears to be unreasonable. Hence the only possible forms for $E_{r,i}$ and E' appear to be

$$E_{r,i} = C \cdot \partial_{x_i} p_r \quad \text{and} \quad E' = C \cdot \sum_{r,i} p_r \partial_{x_i} \tilde{u}_{r,i} \quad (31)$$

(where I have generalized this to three dimensions and n -phases). This is exactly the same form as the $p\delta V$ work terms which exchange energy between the mean flow and internal energy. Note also that the term in the momentum equation must be a divergence so as to conserve momentum.

4 Non-dimensional factor

At this point we are required to specify the form of the non-dimensional factor C . As was discussed above, this term must be sensitive to 1) the presence of a mixed region, and 2) the presence of a shock. Toward this end I first introduce

$$H_i = F_i \sum_r f_r H_r \quad (32)$$

which is the product of two factors. The first F_i will be sensitive to the presence of a shock. The second (the sum) is sensitive to the presence of a mixed region. Specifically

$$H_r = \sum_{s \neq r} f_s \frac{|\rho_r - \rho_s|}{\rho_r + \rho_s} \quad (33)$$

so that $\sum_r f_r H_r$ is just a weighted sum of Atwood numbers. The F_i term is the n^{th} root of a product over phases

$$F_i = [\Pi_r F_{r,i}]^{\frac{1}{n}} \quad \text{where} \quad F_{r,i} = \begin{cases} 0 & \text{iff } \delta u_i < \delta u_l \\ 0.5 \left(\frac{|\delta u_i - \delta u_j|}{\delta \delta u} \right)^{c_{13c}} & \text{iff } \delta u_l < \delta u_i < \delta u_o \\ 1.0 - 0.5 \left(\frac{|\delta u_h - \delta u_i|}{\delta \delta u} \right)^{c_{13c}} & \text{iff } \delta u_o < \delta u_i < \delta u_h \\ 1 & \text{iff } \delta u_h < \delta u_i \end{cases} \quad (34)$$

and

$$\delta u_i = u_{i-\frac{1}{2}} - u_{i+\frac{1}{2}}$$

$$\begin{aligned}
\delta u_o &= c_{13a} \\
\delta \delta u &= c_{13a} \cdot c_{13b} \\
\delta u_l &= \delta u_o - \delta \delta u \\
\delta u_h &= \delta u_o + \delta \delta u
\end{aligned}$$

While the algebra is a little tedious, the function F_i simply implements a smooth transition from zero to one as the relative velocity between two zone edges goes from less than $\delta u_0 = c_{13a}$ to greater than δu_0 . The final result is

$$\begin{aligned}
\partial_t(f_r \rho_r \tilde{u}_{r,i}) + \dots &= \dots c_{10} \partial_{x_i}(f_r p_r H_i) \\
\partial_t(\rho k) + \dots &= \dots c_{10} \sum_{r,i} f_r p_r H_i \partial_{x_i} \tilde{u}_{r,i}
\end{aligned}$$

where c_{10} is a constant. Note that H_i must appear inside one derivative and outside the other so that the resulting combined term in the total energy equation is still a total divergence. The parameters c_{13a} , c_{13b} and c_{13c} have been adjusted to provide reliable shock identification.

It was also found to be necessary to inhibit velocity separation during shocks so as to prevent double counting in this case. This is done by interpolating the $\partial_x p_r$ between the multi-phase value and the single-phase value based on F_i .

5 Modifications to the length scale equation

The length scale equation plays a major (perhaps dominant) role in this model. Because of this and because it will eventually be necessary to introduce an additional source term in it, it is worthwhile to consider in some detail its character and possible motivation. One can trivially write down an equation in one dimension for some conserved scalar quantity l

$$\partial_t l + \partial_x(\bar{u}l) = -\partial_x(D_l \partial_x l) \quad (35)$$

where \bar{u} is some advection velocity and D_l is some diffusion coefficient (presumably needed because of the turbulent character of the flow). If one identifies l with a length scale, then this has the obvious problem that l in the equation decreases in an expansion, whereas we certainly expect the large scale structures in a expansion to grow. Hence the motivation to expand the $\partial_x(\bar{u}l)$ term and reverse the sign on the dilatation part.

$$\partial_t l + \bar{u} \partial_x l = -\partial_x(D_l \partial_x l) + l \partial_x \bar{u} \quad (36)$$

This may, however, overestimate the effects of compression and expansion for two reasons. The first is because of dimensionality. If the flow undergoes an infinitesimal expansion in one direction only, then initially the length scales in the other two directions are not altered. Hence, a more reasonable estimate might be $\frac{1}{3} l \partial_x \bar{u}$ [3].

This consideration might also apply to gradual compressions. However, in gas dynamics compressions are typically discontinuous, i.e., shocks. A shock compression of a mixed region is known to produce additional mix and this requires additional l , not less. In general, one needs to write at least

$$\partial_t l + \bar{u} \partial_x l = -\partial_x (D_l \partial_x l) + c_{lsc} l \partial_x \bar{u} \quad (37)$$

where I have taken $c_{lsc} = 0.3$ if $\partial_x \bar{u} > 0$ and $c_{lsc} = 0$ if $\partial_x \bar{u} < 0$.⁸ The equation is further modified to include the mix region specific advection velocity u_l and a source for l due to the velocity slip S_l [2] (see below for definitions).

$$\partial_t l + (\bar{u} + u_l) \partial_x l = -\partial_x (D_l \partial_x l) + c_{lsc} l \partial_x \bar{u} + S_l \quad (38)$$

It is an indication of the importance of this equation to the overall behavior of the model that without future modification it inhibits the growth of mix due to the Richtmyer-Meshov instability. It was found necessary to add a second source term of the form

$$S_{l2} = c_{lsc} \cdot \frac{\sum_{r>s} f_r f_s \left(\frac{2\rho_{rs}}{\rho_r + \rho_s} \right)^{\frac{1}{2}} (\tilde{w}_s - \tilde{w}_r)}{\sum_{r>s} f_r f_s} \quad (39)$$

This simply mirrors the form of S_l with the \tilde{u}_r 's replaced by \tilde{w}_r 's. It increases the production of l in a mix region which is growing due to turbulent diffusion (as opposed to velocity slip).

6 Final version of the model

The final form of the model (reduced to one dimension) is

$$\begin{aligned} \partial_t f_r + \partial_x (f_r \tilde{u}_r) &= S_{f,r} \\ \partial_t (f_r \rho_r) + \partial_x (f_r \rho_r \tilde{u}_r) &= 0 \\ \partial_t (f_r \rho_r \tilde{u}_r) + \partial_x (f_r \rho_r \tilde{u}_r \tilde{u}_r) &= -f_r \partial_x p_r - \boxed{\text{Reynolds stress}}_{f_r \partial_x T} + \sum_s D_{rs} + \boxed{\text{Shock scattering}}_{c_{10} \partial_x (p_r f_r H)} \\ \partial_t (f_r \rho_r e_r) + \partial_x (f_r \rho_r e_r \tilde{u}_r) &= -h_r p_r \partial_x \bar{u} + S_{e,r} + f_r \epsilon \\ \partial_t (\rho k) + \partial_x (\rho k \bar{u}) &= -\boxed{\text{Reynolds stress}}_{T \partial_x \bar{u}} - \partial_x (\rho D_k \partial_x k) + \sum_{r<s} (\tilde{u}_s - \tilde{u}_r) D_{rs} \\ &\quad + \boxed{\text{Shock scattering}}_{c_{10} \sum_r f_r p_r H \partial_x \tilde{u}_r} - \epsilon \\ \partial_t l + (\bar{u} + u_l) \partial_x l &= -\partial_x (D_l \partial_x l) + \boxed{\text{dilatation}}_{c_{sss} l \partial_x \bar{u}} + S_l + \boxed{\text{turb. source}}_{S_{l2}} \end{aligned} \quad (40)$$

⁸Another interesting possibility would be using $|\partial_x \bar{u}|$ to get an impulsive source of l out of this for shocks.

where:

$$\begin{aligned}
S_{f,r} &= S_{f,r}(e_1, \rho_1, e_2, \rho_2, \dots) && \text{(pressure relaxation scheme - see below)} \\
S_{e,r} &= S_{e,r}(e_1, \rho_1, e_2, \rho_2, \dots) && \text{(pressure relaxation scheme - see below)} \\
p_r &= p_r(\rho_r, e_r) = \frac{1}{1-\gamma} e_r \rho_r && \text{(phase specific pressure)} \\
T &= -\mu_T \frac{4}{3} \partial_x \bar{u} + \frac{2}{3} \rho k, \quad \text{limited by } 0 < T < \frac{5}{4} \rho k && \text{(Reynold's stress)} \\
\mu_T &= \rho \sqrt{k} l_t && \text{(turbulent viscosity)} \\
\rho &= \sum_r f_r \rho_r && \text{(average density)} \\
l_t &= c_2 l && \text{(turbulent length scale)} \\
D_{rs} &= -c_1 \frac{\rho_{rs} f_r f_s}{l} |\Delta_{rs}| \Delta_{rs} && \text{(drag)} \\
\rho_{rs} &= \frac{f_r \rho_r + f_s \rho_s}{f_r + f_s} && \text{(effective average density)} \\
\Delta_{rs} &= (\tilde{u}_r - \tilde{w}_r) - (\tilde{u}_s - \tilde{w}_s) && \text{(velocity difference)} \\
\tilde{w}_{rs} &= -\frac{D}{f_r \rho_r} \partial_x (f_r \rho_r) && \text{(turbulent diffusion velocity)} \\
D &= c_5 \sqrt{k} l_t && \text{(turbulent diffusion coefficient)} \\
H &= && \text{(shock scattering - see eqn. 32)} \\
h_r &= \frac{f_r / (\rho_r c_r^2)}{\sum_s (f_s / (\rho_s c_s^2))} && \text{(relative compressibility)} \\
c_r &= && \text{sound speed in phase } r \\
\bar{u} &= \sum_r f_r \tilde{u}_r && \text{(volume average velocity)} \\
\varepsilon &= c_4 \frac{\rho k^{3/2}}{l_t} && \text{(turbulent dissipation)} \\
D_k &= c_7 \sqrt{k} l_t && \text{(diffusion of turbulence)} \\
u_l &= \frac{\sum_{r>s} f_r f_s (f_r - f_s) (\tilde{u}_s - \tilde{u}_r)}{\sum_{r>s} f_r f_s} && \text{(length scale advection velocity)} \\
D_l &= c_8 \sqrt{k} l_t && \text{(length scale diffusion)} \\
S_l &= c_{lsc} \cdot \frac{\sum_{r>s} f_r f_s \left(\frac{2\rho_{rs}}{\rho_r + \rho_s} \right)^{1/2} (\tilde{u}_s - \tilde{u}_r)}{\sum_{r>s} f_r f_s} && \text{(length scale source - slip)} \\
S_{l2} &= c_{lsc2} \cdot \frac{\sum_{r>s} f_r f_s \left(\frac{2\rho_{rs}}{\rho_r + \rho_s} \right)^{1/2} (\tilde{w}_s - \tilde{w}_r)}{\sum_{r>s} f_r f_s} && \text{(length scale source - diffusion)}
\end{aligned}$$

The relaxation terms $S_{f,r}$ and $S_{e,r}$ allows phases occupying the same zone to exchange volume fraction and internal energy ($\sum_r S_{f,r} = \sum_r S_{e,r} = 0$) at a rate inversely proportional to the length scale l . As has been indicated previously, this is derived from the work of Youngs[2, 3, 4]. Deviations from that work are indicated in the boxes. They

parameter	value	what
c_1	$7.25 - 5.25 \cdot At$	drag
c_2	0.075	turbulent length scale w.r.t. l
c_4	0.09	dissipation of turbulence kinetic energy
c_5	2.0	mass diffusion
c_7	1.0	turbulent kinetic energy diffusion
c_8	2.0	length scale diffusion
c_{10}	2.0	shock scattering
c_{11}	0.005	mix trigger
$c_{13a,b,c}$	5 [m/s], 0.4, 1.2	shock finder
c_{sss}	0.0 / 0.3	dilatation
c_{lsc}	1.0	length scale source due to velocity slip
c_{lsc2}	1.0	length scale source due to diffusion

Figure 4: Parameters used in the model.

fall into four groups.

- Shock scattering terms (proportional to c_{10}) appear in the momentum and k -equations.
- Reynolds stress terms of a different sort also appear in these two equations. Note the need for a limiter on T .
- The definition of \bar{u} as it appears in the $p\delta V$ work term in the energy equation has been changed. This allows a “bad” term to be deleted from the k -equation as discussed above.
- Two length scale source terms in the length scale equation are changed.
- I have dropped the added mass terms.

The parameters of the model are show in Table 4. The origin of the values of c_1 , c_{10} , c_{sss} , and c_{lsc2} are described in the text. The remaining values are from ref. [2] and ref. [3]. The model has been implemented as part of a one-dimensional Lagrangian hydrocode.

7 Comparisons to experiment

This effort was originally motivated by the inability of the model to handle heavy to light RMI. This section makes comparisons to three experiments. Since the changes

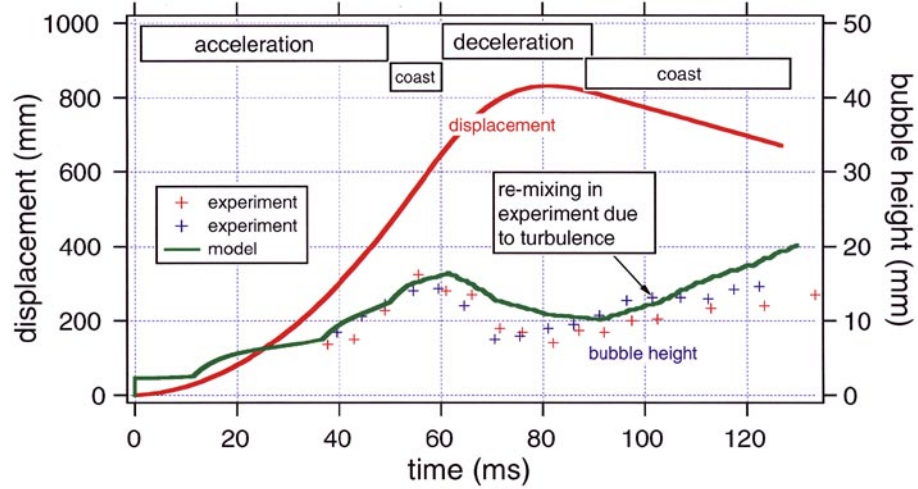


Figure 5: The figure shows a comparison between the measured and modeled bubble height amplitudes from the acceleration-deceleration experiment. The model results are shown in green. The experimental data appears as red and green points. Reasonable agreement is obtained. The red curve shows the displacement of the interface as a function of time.

(particularly those to the length scale sources) will change the behavior of the model in general, a comparison is made to an acceleration/deceleration “rocket rig” experiment. The second is a heavy to light reshock experiment in which improved behavior is observed. A reasonable agreement with the data is obtained, with the two experiments together substantially constraining the model. Lastly the model is compared to the experiment of Poggi et al.[13]. Reasonable agreement is obtained with the turbulence production measured in that experiment.

7.1 Acceleration - Deceleration

The acceleration / deceleration experiment of Smeeton and Youngs [12] used immiscible fluids in the “rocket rig” facility at AWE. The tank first experienced a constant acceleration, followed by a coast, followed by a more or less constant deceleration, followed by another coast. The turbulent mixing layer was observed to first grow, then demix during the deceleration, and then resume growing during the final coast phase. This subsequent regrowth is interpreted as being due to the turbulence [12].

The two fluids (actually a calcium chloride solution and hexane, densities of 1.142

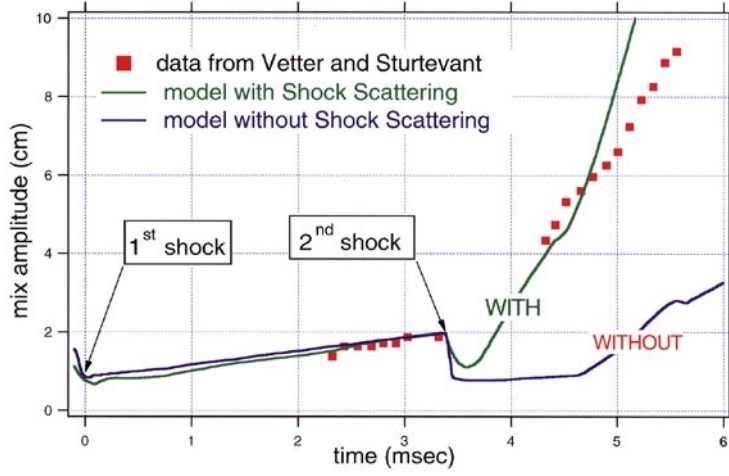


Figure 6: The figure shows a comparison between the measured and modeled values of the total mix width in the Vetter and Sturtevant experiment. The red points are from the experiment. The green and blue solid lines show the results of the model with and without the shock scattering. Reasonable agreement is obtained with the modified model up until the arrival of the reflected rarefaction at about 4.5 msec. The unmodified model produces no additional mix due to the reshock.

g/cm^2 and 0.66 g/cm^2) are modeled with a scaled ideal gas equation-of-state. The initial temperature distribution through the problem is set to produce the pressure gradient required to give a uniform initial acceleration. Subsequent changes in the acceleration are implemented through changes to the external pressure boundary conditions and necessarily produce a series of small shocks (below the threshold for the shock finder). The results of the simulation are compared to the experiment in Fig. 5. Reasonable agreement is obtained. In this case the initial mix was triggered by taking l in the drag term to be the greater of the actual l or $c_{11} \cdot \Delta x$ where Δx is the zone size.

This is a significant experiment because it tests not only the multiphase flow part of the model, but also the kl turbulence part. A substantial effort was required to find parameters which would simultaneously fit both this experiment and the reshock experiment (see below). The nature of the difficulty is as follows. The length scale l is a sort of quasi-conserved quantity. I.e., just because one would like more $\int l dx$, does not mean the terms on the right-hand side will produce it. In order to grow the mix region, the model must increase $\int l dx$. In the case of the RTI, the S_l term generates the required l . In the current case the S_{l2} term was added to enable the growth of the mixing region in the reshock experiment. It does this by allowing turbulence to generate l after the passage of the shock. While it appears possible to match the reshock experiment with a variety of values of c_{10} and c_{lsc2} (they are anti-correlated), not perturbing the accel-

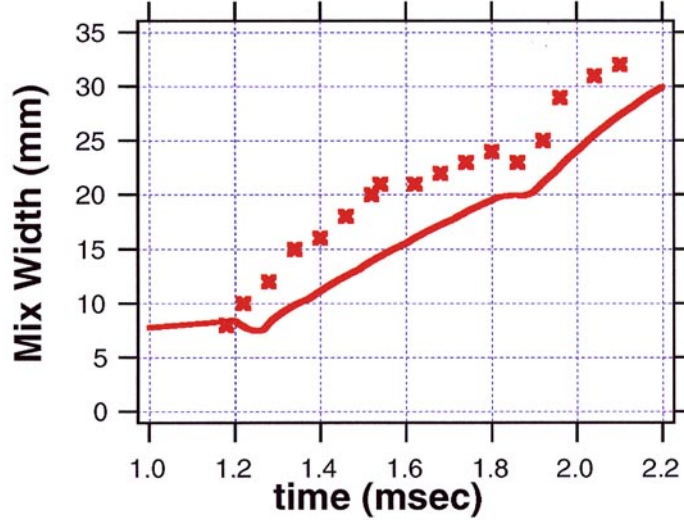


Figure 7: The figure shows a comparison between the total mix width in the reshock experiment of Poggi et al. and the model. The first reshock occurs at about 1.2 msec. The model modestly underestimates the width when it is run using the parameters from the previous two experiments. (An additional shock arrives at about 1.9 msec and produces additional growth in the mix region.)

eration / deceleration experiment is more difficult. This experiment sets an upper limit on the value of c_{lsc2} (larger values produce too much mix at late times). The resulting value of $c_{l0} = 2$ appears large in that it implies that the energy removed from the main flow and moved into k is similar to that moved into internal energy.⁹ If the change in k produced by the passage of the shock is, in fact, too big, then another mechanism for producing l may be required.

7.2 Reshock

The reshock experiment of Vetter and Sturtevant [11] provides a test of the ability of the model to produce mix when a shock propagates through a mixed region in the RT stable direction. In this air-SF₆ Mach 1.5 shock tube experiment the initial interface is formed by a membrane. The incident shock brakes the membrane and then is reflected from the end wall (62 cm from the initial interface location). This reflection (a heavy to light shock) accelerates the interface approximately 3.4 msec. after the initial shock

⁹Recall that $\sum_r f_r H_{r,i}$ cannot be greater than $\frac{1}{4}$. At in the two phase case, for instance.

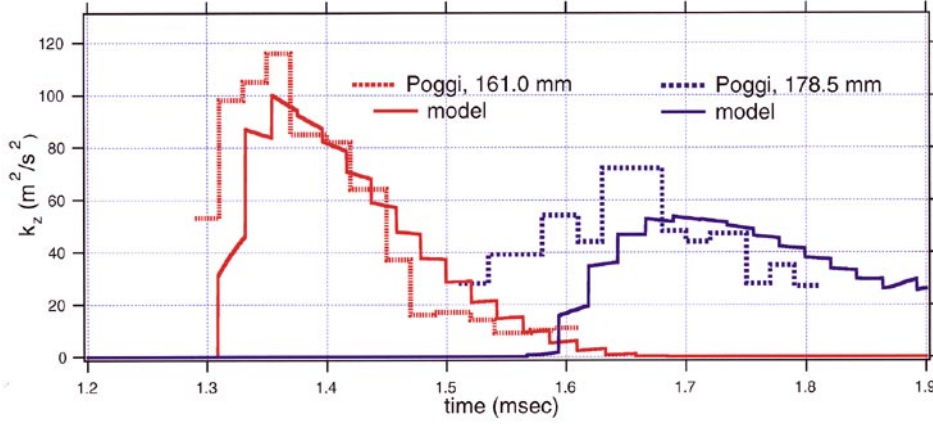


Figure 8: The figure shows a comparison between the velocity fluctuations as measured in the Poggi et al. experiment and in the model. Reasonable agreement is obtained with respect to the amplitude. The timing shifts are discussed in the text.

and is observed to cause a substantial growth in the mixing rate.

Because of the poorly defined initial conditions provided by the membrane, no claim is made as to the modeling of the initial interaction. Rather, the initial conditions in the model (l at the interface) are adjusted to match the measured mix width before the reshock (at about 3 msec.). The subsequent reshock is then modeled and used to constrain parameters. The simulation of this experiment is carried out with ideal gas equations-of-state ($\gamma = 1.402$ for air and $\gamma = 1.0935$ for SF_6). The results are compared to the experiment in Fig. 6. Good agreement is obtained up until the arrival of a reflected rarefaction at 4.5 msec. (The mix trigger (c_{11}) is not used here.) The behavior of the unmodified model is also shown.

7.3 Reshock with measurement of $k_i = \overline{\rho u_i'' u_i''}$

The experiment of Poggi et al.[13] resembles that of Vetter and Sturtevant and has been modeled in a similar manner. In addition to mix width, it also provides data on the value of the velocity fluctuations $k_i = \overline{\rho u_i'' u_i''}$. The Poggi experiment differs from Vetter and Sturtevant in that the positions of the air and the SF_6 where reversed, the test section is shorter (30 cm), and the Mach number of 1.45 is slightly lower. Comparisons to the total mix width and to k_x are shown in figures 7 and 8 respectively. Because the model does not account for anisotropies in k , the model quantity plotted is $k_x = k/3$. I.e., the model assumes isotropy ($k_x = k_y = k_z$ and $k = k_x + k_y + k_z$). Because the Poggi experiment saw large anisotropies in k_i , it is likely that the model is removing about two times as much energy from the mean flow as it should.

8 Conclusions and Outlook

This paper has proposed an innovative method to improve the behavior of an existing model for the mix from combined RMI and RTI. The model was first tuned to the variable acceleration Rayleigh-Taylor experiment of Smeeton and Youngs and the reshock experiment of Vetter and Sturtevant. Subsequent comparisons to the experimental data from the Poggi experiment are in reasonable agreement.

Issues which require further investigation include the scaling of the turbulence production in the model with Mach number and Atwood number (and subsequent comparisons to experiments or simulations). A further examination of the modifications to the l equation is also planned.

9 Acknowledgements

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